On completeness of description of an equilibrium canonical ensemble by reduced s-particle distribution function

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Abstract. In this article it is shown that in a classical equilibrium canonical ensemble of molecules with s-body interaction full Gibbs distribution can be uniquely expressed in terms of a reduced s-particle distribution function. This means that whenever a number of particles N and a volume V are fixed the reduced s-particle distribution function contains as much information about the equilibrium system as the whole canonical Gibbs distribution. The latter is represented as an absolutely convergent power series relative to the reduced s-particle distribution function. As an example a linear term of this expansion is calculated. It is also shown that reduced distribution functions of order less than s don't possess such property and, to all appearance, contain not all information about the system under consideration.

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1. Introduction

In classical statistical mechanics an equilibrium system of N molecules in a volume V is described by canonical distribution function $F_N(q,p)$, where (q,p) is a set of phase variables: coordinates q_i and momenta p_i of molecules. If interaction of molecules is additive, reduced distribution functions are introduced [1, 2]. They are used for evaluation of thermodynamic characteristics of such molecular system. It's usually accepted that reduced distribution functions contain information about a molecular system less than the canonical Gibbs distribution function. It's also supposed that the lower an order of a reduced distribution function is, the less information it contains. But there does not exist a proof of this statement in scientific literature.

On the other hand, it is known that for an equilibrium canonical ensemble of non-interacting particles a canonical distribution function $F_N(q,p)$ is decomposed into a product of reduced one-particle distribution functions $F_1(q,p)$ [1]. This means that all information about such system is contained in the reduced one-particle distribution function. In [3, 4] it was proved that for a closed molecular system with pair interaction there is a one-to-one correspondence between a canonical distribution and a reduced two-particle distribution function.

In this paper it's proved that for a system having interaction potentials up to order s there exists one-to-one correspondence between full canonical distribution function and a reduced s-particle distribution function. This means that the s-particle function contains the whole information about system under consideration.

We consider an equilibrium system of N particles contained in the volume V under the temperature T. Potential energy of system is supposed to have the form

$$U_N(q_1,\ldots,q_N)=\sum_{l=1}^{s}\sum_{1\le j_1<\cdots<j_l\le N}u_l(q_{j_1},\ldots,q_{j_l}), \tag{1}$$

where s is an arbitrary fixed integer less than N and $u_l(q_1,\ldots,q_l)$ is a direct interaction energy of l particles. Probability distribution function of equilibrium system is the canonical Gibbs distribution which is decomposed into a product of a momentum distribution function and a configurational one [1, 2]. The former is expressed as a product of one-particle Maxwell distributions, the latter has the form

$$D_N(q_1,\ldots,q_N)=Q_N^{-1}\exp\{-\beta U_N(q_1,\ldots,q_N)\}, \tag{2}$$

where $\beta=1/kT$, k is the Boltzmann constant and Q_N is the configuration integral

$$Q_N=\int\exp\{-\beta U_N(q_1,\ldots,q_N)\}dq_1\cdots dq_N. \tag{3}$$

Here and below integrating with respect to every configurational variable is carried out over the volume V. For a system having interaction of form (1) reduced distribution functions are introduced by expressions [1]

$$F_l(q_1,\ldots,q_l)=\frac{N!}{(N-l)!}\int D_N(q_1,\ldots,q_N)dq_{l+1}\cdots dq_N,\quad l=1,2,\ldots. \tag{4}$$

These functions are used instead of full canonical distribution (2) to calculate various characteristics of the molecular system. Let us investigate properties of the reduced s-particle distribution function.

Potential energy (1) can be written as

$$U_N(q_1,\ldots,q_N) = \sum_{1\le j_1<\cdots<j_s\le N} \phi(q_{j_1},\ldots,q_{j_s}), \tag{5}$$

where

$$\phi(q_1,\ldots,q_s) = \sum_{r=1}^{s} (C_{N-r}^{s-r})^{-1} \sum_{1\le j_1<\cdots<j_r\le s} u_r(q_{j_1},\ldots,q_{j_r}) \tag{6}$$

and $C_m^n = m!/\{n!(m-n)!\}$ are binomial coefficients.

Introduce a function $h(q_1,\ldots,q_s)\}$ by the relation

$$\exp\{-\beta\phi(q_1,\ldots,q_s)\} = \sigma\{1+h(q_1,\ldots,q_s)\}, \tag{7}$$

where

$$\sigma = \frac{1}{V^s}\int \exp\{-\beta\phi(q_1,\ldots,q_s)\}\, dq_1\cdots dq_s. \tag{8}$$

The canonical Gibbs distribution (2) takes the form

$$D_N(q_1,\ldots,q_N) = Q_N^{-1} \prod_{1\le j_1<\cdots<j_s\le N} [1+h(q_{j_1},\ldots,q_{j_s})] \tag{9}$$

with

$$Q_N = \int \prod_{1\le j_1<\cdots<j_s\le N} [1+h(q_{j_1},\ldots,q_{j_s})]\, dq_1\cdots dq_N. \tag{10}$$

From (9) and (10) it follows that statistical properties of system under consideration are completely determined by the specifying single function of s configurational variables $h(q_1,\ldots,q_s)$ and two external parameters N and V. The assumption naturally arises that another single function of s configurational variables $F_s(q_1,\ldots,q_s)$ can completely determine all statistical properties of this system. It turns out that this is indeed the case and reduced distribution function of order s plays a special role among all reduced functions (4). It can be proved that canonical Gibbs distribution (2) is expressed in terms of $F_s(q_1,\ldots,q_s)$. This means that there is one-to-one correspondence between D_N and F_s. Therefore the system under consideration can be completely described by both canonical distribution and reduced s-particle distribution function. All functions (4) are expressed in terms of $F_s(q_1,\ldots,q_s)$ too. We prove these statements below. That proof is analogous to one for system with two-body interaction ($s=2$) presented in the papers [3, 4].

In section 2 we pose a mathematical problem for our molecular system and formulate conditions for existence and uniqueness of its solution. In section 3 feasibility of these conditions for considered physical system are proved. In section 4 an expression for function $h(q_1,\ldots,q_s)$ in terms of $F_s(q_1,\ldots,q_s)$ is calculated. In section 5 an expression for the canonical distribution in terms of reduced s-particle distribution function is produced. In section 6 it is shown that reduced distribution functions of orders less then s don't possess such property.

2. Mathematical formulation of problem

Let us introduce a function $f(q_1, \ldots, q_s)$ by the relation

$$F_s(q_1, \ldots, q_s) = \frac{N!}{(N-s)!\, V^s}[1 + f(q_1, \ldots, q_s)]. \tag{11}$$

Both the function $f(q_1, \ldots, q_s)$ and the function $h(q_1, \ldots, q_s)$ satisfy the conditions

$$\int f(q_1, \ldots, q_s)\, dq_1 \cdots dq_s = 0, \qquad \int h(q_1, \ldots, q_s)\, dq_1 \cdots dq_s = 0. \tag{12}$$

From expressions (4), (9), and (11) it follows that

$$1 + f(q_1, \ldots, q_s) = \frac{V^s}{Q_N} \int \prod_{1 \le j_1 < \cdots < j_s \le N} [1 + h(q_{j_1}, \ldots, q_{j_s})] dq_{s+1} \cdots dq_N. \tag{13}$$

This relation defines the transformation $\{h \to f\}$ and can be considered as a nonlinear equation relative to $h(q_1, \ldots, q_s)$. If there exists a solution $h(q_1, \ldots, q_s; [f])$ of this equation then the function $D_N(q_1, \ldots, q_N)$ becomes an operator function of f. It means that both the canonical Gibbs distribution D_N and all reduced distribution functions F_l are expressed in terms of the single reduced distribution function F_s. Thus we have to prove that equation (13) has a unique solution and therefore the transformation $\{h \to f\}$ has inverse one $\{f \to h\}$.

Multiplying equation (13) by $Q_N V^{-N}$ and using (10) we rewrite it in the form

$$[1 + f(q_1, \ldots, q_s)] \frac{1}{V^N} \int \prod_{1 \le j_1 < \cdots < j_s \le N} [1 + h(p_{j_1}, \ldots, p_{j_s})]\, dp_1 \cdots dp_N$$
$$- \frac{1}{V^{N-s}} \int \prod_{1 \le j_1 < \cdots < j_s \le N} [1 + h(q_{j_1}, \ldots, q_{j_s})] dq_{s+1} \cdots dq_N = 0. \tag{14}$$

The left-hand side of (14) is a polynomial operator of degree $\mathcal{N} = C_N^s$ relative to h and of degree one relative to f. Denote this operator by $\mathcal{F}(h, f)$. Equation (14) can be written in a symbolic form

$$\mathcal{F}(h, f) = 0. \tag{15}$$

To solve this equation it is necessary to specify an additional condition

$$\mathcal{F}(h^{(0)}, f^{(0)}) = 0, \tag{16}$$

where $f^{(0)}(q_1, \ldots, q_s)$ and $h^{(0)}(q_1, \ldots, q_s)$ are assigned functions.

We can easily determine these functions for our physical system. If the external field and all interactions between particles are absent, i.e., all potentials u_l are constant, then the function $h(q_1, \ldots, q_s)$ vanishes. Under this condition $Q_N = Q_N^{(0)} = V^N$, $D_N(q_1, \ldots, q_N) = D_N^{(0)} = V^{-N}$, and $f(q_1, \ldots, q_s) = 0$. Therefore we can take $h^{(0)} = 0$ and $f^{(0)} = 0$ in (16)

Equation (15) and additional condition (16) form a problem on implicit function. In functional analysis there is a number of theorems on implicit function for operators of various smoothness classes. We use the theorem for analytic operator in Banach space in the form given in the book [5]

Theorem. (On implicit function). *Let $\mathcal{F}(h, f)$ be an analytic operator in $D_r(h^{(0)}, E_1) \times D_\rho(f^{(0)}, E)$ with values in E_2. Let an operator $B \stackrel{\mathrm{def}}{=} -\partial\mathcal{F}(h^{(0)}, f^{(0)})/\partial h$ have a bounded inverse one. Then there are positive numbers ρ_1 and r_1 such that a unique solution $h = \chi(f)$ of the equation $\mathcal{F}(h, f) = 0$ with the additional condition $\mathcal{F}(h^{(0)}, f^{(0)}) = 0$ exists in a solid sphere $D_{r_1}(h^{(0)}, E_1)$. This solution is defined in a solid sphere $D_{\rho_1}(f^{(0)}, E)$, is analytic there, and satisfies the condition $h^{(0)} = \chi(f^{(0)})$.*

Here $D_r(x_0, \mathcal{E})$ denotes a solid sphere of radius r in a neighborhood of the element x_0 in a normalized space $\mathcal{E}$, the symbol $\times$ denotes the Cartesian product of sets, $\partial\mathcal{F}/\partial h$ is Fréchet derivative [5, 6] of the operator $\mathcal{F}$, $h^{(0)}$ and $f^{(0)}$ are assigned elements of the respective spaces E_1 and E. If the functions $h(q_1, \ldots, q_s)$ and $f(q_1, \ldots, q_s)$ satisfy this theorem conditions, the former is a single valued operator function of the later.

To prove an existence and uniqueness of a solution of problem (15), (16) we have to show that all conditions of the above theorem are satisfied.

3. Proof of feasibility of the theorem conditions

First we define spaces E_1, E, and E_2 mentioned in the theorem for functions describing the physical system under consideration.

3.1. Functional spaces of problem

Potentials $u_k(q_1, \ldots, q_k)$ are real symmetric functions. Suppose they are bounded below for almost all $\{q_1, \ldots, q_k\} \in V$. All physically significant potentials possess this property. Under this condition integral (8) exists and $h(q_1, \ldots, q_s)$ is a real symmetric function bounded for almost all $\{q_1, \ldots, q_s\} \in V$.

A set of functions bounded nearly everywhere forms a complete linear normalized space (Banach space) with respect to the norm [6, 7]

$$\|h\| = \operatorname*{vrai\,sup}_{\{q_1, \ldots, q_s\} \in V} |h(q_1, \ldots, q_s)| \,, \tag{17}$$

where "vrai sup" denotes an essential upper bound of the function on the indicated set. It is called the space of essentially bounded functions and is denoted by $L_\infty(\mathcal{V}^{(s)})$. Here $\mathcal{V}^{(s)} \stackrel{\mathrm{def}}{=} V \times \cdots \times V$ is a repeated s times Cartesian product of V by itself. In addition $h(q_1, \ldots, q_s)$ satisfies condition (12). The set of such functions is a subspace of $L_\infty(\mathcal{V}^{(s)})$. It is easy to show that this subspace is a complete space relative to norm (17). Therefore we can take the Banach space of symmetric essentially bounded functions satisfying condition (12) as E_1.

Expression (13) for $f(q_1, \ldots, q_s)$ includes multiple integrals of different power combinations of $h(q_1, \ldots, q_s)$. Any power of essentially bounded function are integrable with respect to arbitrary set of variables $\{q_{j_1}, \ldots, q_{j_r}\}$ over V [8]. Therefore all integrals in (14) are essentially bounded functions too. Arguing as above, we can show that the space E of functions $f(q_1, \ldots, q_s)$ coincides with E_1. Continuing in the same way we

can show that E_2 is the same space. Thus we define the spaces of the above theorem as $E = E_1 = E_2 = L_\infty(\mathcal{V}^{(s)})$ with property (12).

From (7) and (11) for $h(q_1, \dots, q_s)$ and $f(q_1, \dots, q_s)$ it follows that $f > -1$ and $h > -1$. Therefore we can take a manifold $\{f > -1,\ h > -1\}$ as a definition domain of the operator $\mathcal{F}(h, f)$. Since the left-hand side of (14) is a polynomial, the operator $\mathcal{F}(h, f)$ is analytical in this domain. As stated above the additional condition (16) is valid for $h^{(0)} = f^{(0)} = 0$. Thus any solid spheres of E_1, E with centers at $h^{(0)} = 0$, $f^{(0)} = 0$ and radii $r < 1$, $\rho < 1$ respectively can be used as domains $D_r(h^{(0)}, E_1)$ and $D_\rho(f^{(0)}, E)$ indicated in the theorem.

Finally it is necessary to prove that the operator

$$B \stackrel{\text{def}}{=} -\frac{\partial \mathcal{F}(h, f)}{\partial h}\bigg|_{\substack{h=0,\\ f=0}} \tag{18}$$

has a bounded inverse one.

3.2. Properties of the operator B

To find the inverse operator B^{-1} it is necessary to solve the equation $Bh = y$, where $h \in E_1$, $y \in E_2$. The expression for Bh is a linear relative to h part in the left-hand side of relation (14) as $f = 0$. Expanding products in (14) and keeping linear summands we obtain

$$(Bh)(q_1, \dots, q_s)) = \frac{1}{V^{N-s}} \int \sum_{1 \le j_1 < \dots < j_s \le N} h(q_{j_1}, \dots, q_{j_s}) dq_{s+1} \cdots dq_N. \tag{19}$$

Variables $\{q_{j_1}, \dots, q_{j_s}\}$ are divided into two groups $\{q_{j_1}, \dots, q_{j_l}\}$ and $\{q_{j_{l+1}}, \dots, q_{j_s}\}$ for $l \le s$, where $(j_1, \dots, j_l) \subset (1, \dots, s)$ and $(j_{l+1}, \dots, j_s) \subset (s+1, \dots, N)$. The sum in the right-hand side of (19) is divided into two parts for each $0 \le l \le s$. The expression (19) can be rewritten in the form

$$(Bh)(q_1, \dots, q_s) = \sum_{l=0}^{s} \sum_{1 \le j_1 < \dots < j_l \le s} \sum_{s+1 \le j_{l+1} < \dots < j_s \le N} \cdot \frac{1}{V^{N-s}} \int h(q_{j_1}, \dots, q_{j_l}, q_{j_{l+1}}, \dots, q_{j_s}) dq_{s+1} \cdots dq_N. \tag{20}$$

We suppose that $s < N/2$. Integration in (20) is carried out with respect to variables from second group $\{q_{j_{l+1}}, \dots, q_{j_s}\} \subset \{q_{s+1}, \dots, q_N\}$ and remaining ones $\{q_{s+1}, \dots, q_N\} \backslash \{q_{j_{l+1}}, \dots, q_{j_s}\}$. Here a symbol $\backslash$ denotes difference of sets. Since the function $h(q_1, \dots, q_s)$ is symmetric, we see that the summation with respect to $(j_{l+1}, \dots, j_s)$ gives C_{N-s}^{s-l} identical terms. In the result we get

$$(Bh)(q_1, \dots, q_s) = \sum_{l=1}^{s} C_{N-s}^{s-l} \sum_{1 \le j_1 < \dots < j_l \le s} \cdot \frac{1}{V^{s-l}} \int h(q_{j_1}, \dots, q_{j_l}, p_1, \dots, p_{s-l}) dp_1 \cdots dp_{s-l}. \tag{21}$$

Here we omitted summands with $l = 0$ because of property (12) for the function h.

It's easy to estimate a norm of the operator B. Using definition (17) we obtain

$$\|Bh\| \leq \sum_{l=1}^{s} C_{N-s}^{s-l} \sum_{1\leq j_1<\cdots<j_l\leq s} \|h\|$$
$$= \sum_{l=1}^{s} C_{N-s}^{s-l} C_s^l \|h\| = (C_N^s - C_{N-s}^s)\|h\|. \tag{22}$$

From here we get an estimation

$$\|B\| \leq (C_N^s - C_{N-s}^s). \tag{23}$$

Thus the operator B is bounded.

To simplify transformations we introduce notation

$$\overline{h}^{(k)}(q_1,\ldots,q_k) = \frac{1}{V^{s-k}} \int h(q_1,\ldots,q_s)dq_{k+1}\cdots dq_s. \tag{24}$$

Using (21) and (24) we can write the equation $Bh = y$ in the next form

$$\sum_{l=1}^{s} C_{N-s}^{s-l} \sum_{1\leq j_1<\cdots<j_l\leq s} \overline{h}^{(l)}(q_{j_1},\ldots,q_{j_l}) = y(q_1,\ldots,q_s). \tag{25}$$

Integrating this equation wit respect to q_s, then q_{s-1} and so on we obtain a system of equations for $\overline{h}^{(k)}$

$$\sum_{l=1}^{k} C_{N-k}^{s-l} \sum_{1\leq j_1<\cdots<j_l\leq k} \overline{h}^{(l)}(q_{j_1},\ldots,q_{j_l}) = \overline{y}^{(k)}(q_1,\ldots,q_k) \tag{26}$$

for all$k = 1,\ldots,s$. Correctness of this expression for arbitrary k is easily tested by induction. Note that $\overline{h}^{(0)} = 0$ and $\overline{h}^{(s)} = h$.

A solution of system (26) is obtained step by step starting from the first equation with $k = 1$. It has the form

$$\overline{h}^{(k)}(q_1,\ldots,q_k) = \frac{1}{C_{N-k}^{s-k}} \sum_{r=1}^{k} (-1)^{k-r} \frac{C_{N-k}^{s-k+1}}{C_{N-r}^{s-k+1}} \sum_{1\leq j_1<\cdots<j_r\leq k} \overline{y}^{(r)}(q_{j_1},\ldots,q_{j_r}) \tag{27}$$

for all $k = 1,\ldots,s$. This solution is easily checked by forward substitution into system (26).

Putting here $k = s$ we obtain the expression for the inverse operator B^{-1}

$$h(q_1,\ldots,q_s) = (B^{-1}y)(q_1,\ldots,q_s)$$
$$= \sum_{r=1}^{s} (-1)^{s-r} \frac{N-s}{N-r} \sum_{1\leq j_1<\cdots<j_r\leq s} \overline{y}^{(r)}(q_{j_1},\ldots,q_{j_r}). \tag{28}$$

From here it's easy to estimate the norm of the inverse operator B^{-1}. Evaluate the norm of right-hand-side of (28)

$$\|B^{-1}y\| \leq \sum_{r=1}^{s} \frac{N-s}{N-r} \sum_{1\leq i_1<\cdots<i_r\leq s} \|y\| = \sum_{r=1}^{s} \frac{N-s}{N-r} C_s^r \|y\|. \tag{29}$$

We obtain from here

$$\|B^{-1}\| \le \sum_{r=1}^{s} \frac{N-s}{N-r} C_s^r \le 2^s - 1. \tag{30}$$

Therefore the operator B^{-1} exists and it is bounded.

So all conditions of the above theorem are valid for our physical system. Hence there exists a unique solution h of problem (15), (16) as a function of f. This solution defines an inverse transformation from the function f to the function h: $h(q_1,\dots,q_s) = h(q_1,\dots,q_s;[f])$.

4. Derivation of the inverse transformation $h(f)$

To obtain the transformation $f \to h$ we have to solve equation (14) relative to $h(q_1,\dots,q_s)$. At first define an auxiliary operator function $g(h)$ by means of a relation

$$\frac{1}{V^{N-s}} \int \prod_{1\le j_1<\dots<j_s\le N} [1 + h(q_{j_1},\dots,q_{j_s})] dq_{s+1}\cdots dq_N = 1 + g(h). \tag{31}$$

This operator function is a polynomial of degree $\mathcal{N} = C_N^s$ relative to h and depends on s configurational variables $\{q_1,\dots,q_s\}$. It can be written in the form

$$g(h) = \sum_{l=1}^{\mathcal{N}} g_l(h), \tag{32}$$

where $g_l(h)$ is a uniform operator of order l relative to h. Let us derive the expression for $g_l(h)$ from (31).

For the sake of abbreviation of subsequent calculations we introduce next notations. We will denote by number $K \in (1,\dots,\mathcal{N})$ every ordered collection $(j_1,\dots,j_s) \subset (1,\dots,N)$. Such one-to-one correspondence can be always made. A collection $(q_{j_1},\dots,q_{j_s})$ is an element of manifold $\mathcal{V}^{(s)}$. We will denote this element by X_K. By definition put $X_1 = (q_1,\dots,q_s)$.

Expanding the product in (31) we obtain for every $l = 1,\dots,\mathcal{N}$

$$g_l(h) = \frac{1}{V^{N-s}} \int dq_{s+1}\cdots dq_N \sum_{1\le K_1<\dots<K_l\le\mathcal{N}} h(X_{K_1})\cdots h(X_{K_l}). \tag{33}$$

Introduced operators $g(h)$ and $g_l(h)$ are symmetrical functions of s configurational variables: $g(h) = g(q_1,\dots,q_s;[h])$ and $g_l(h) = g_l(q_1,\dots,q_s;[h])$. In contrast to h and f both $g(q_1,\dots,q_s;[h])$ and $g_l(q_1,\dots,q_s;[h])$ don't satisfy condition (12) except for $g_1(q_1,\dots,q_s;[h])$. First term of series (32) is $g_1(h) = Bh$ and satisfies to condition (12). Configuration integral (10) takes the form

$$Q_N = V^N[1 + \overline{g}^{(0)}] = V^N[1 + \sum_{k=2}^{\mathcal{N}} \overline{g}_k^{(0)}]. \tag{34}$$

Here we used notation (24).

Substituting definitions (31) and (34) into (14) we write it in the form

$$(1+f)[1 + \overline{g}^{(0)}(h)] - [1 + g(h)] = 0, \tag{35}$$

where f and $g(h)$ are functions of $X_1 = (q_1, \ldots, q_s)$. But value $\overline{g}^{(0)}$ doesn't depend on configurational variables. It is a functional relative h. Substituting here expansions (32) and (34) we reduce this equation to the form

$$f[1 + \sum_{l=2}^{\mathcal{N}} \overline{g}_l^{(0)}(h)] + \sum_{l=2}^{\mathcal{N}} [\overline{g}_l^{(0)}(h) - g_l(h)] - Bh = 0. \tag{36}$$

Here we have taken into account that $g_1(h) = Bh$ and $\overline{g}_1^{(0)}(h) = 0$.

For subsequent calculation we need multilinear operators

$$G_l(y_1, \ldots, y_l) = \frac{1}{V^{N-s}} \int dq_{s+1} \cdots dq_N \sum_{1 \le K_1 < \cdots < K_l \le \mathcal{N}} y_1(X_{K_1}) \cdots y_l(X_{K_l}). \tag{37}$$

These operators are linear with respect to any functional argument y_i. We can consider the operator functions $g_l(h)$ as generated by these multilinear operators G_l

$$g_l(h) = G_l(h, \ldots, h). \tag{38}$$

Operators $G_l(y_1, \ldots, y_l)$ are functions of configurational variables $(q_1, \ldots, q_s) = X_1$. In general these functions aren't symmetrical relative to $(q_1, \ldots, q_s)$. But this isn't important since under substituting of these operator functions into equation (36) symmetric property will be hold automatically. In the result we can rewrite equation (36) as

$$h = B^{-1} f [1 + \sum_{l=2}^{\mathcal{N}} \overline{G}_l^{(0)}(h, \ldots, h)] + B^{-1} \sum_{l=2}^{\mathcal{N}} [\overline{G}_l^{(0)}(h, \ldots, h) - G_l(h, \ldots, h)]. \tag{39}$$

We will search a solution of this equation in the form of power series

$$h = \sum_{k=1}^{\infty} h_k(f), \tag{40}$$

where $h_k(f)$ are uniform operators of order k relative to f. At the same time they are functions of configurational variables X_i. Substituting (40) into (39) and taken into account linearity of $G_l(y_1, \ldots, y_l)$ with respect to any argument y_i we obtain

$$\sum_{k=1}^{\infty} h_k(f) = B^{-1} f + B^{-1} \sum_{l=2}^{\mathcal{N}} \sum_{j_1=1}^{\infty} \cdots \sum_{j_l=1}^{\infty} \overline{G}_l^{(0)}(h_{j_1}, \ldots, h_{j_l}) f + B^{-1} \sum_{l=2}^{\mathcal{N}} \sum_{j_1=1}^{\infty} \cdots \sum_{j_l=1}^{\infty} [\overline{G}_l^{(0)}(h_{j_1}, \ldots, h_{j_l}) - G_l(h_{j_1}, \ldots, h_{j_l})]. \tag{41}$$

Transform sums over $j_1, \ldots, j_l$ as follows

$$\sum_{j_1=1}^{\infty} \cdots \sum_{j_l=1}^{\infty} = \sum_{k=l}^{\infty} \sum_{j_1 + \cdots + j_l = k} . \tag{42}$$

Then relation (41) takes the form

$$\sum_{k=1}^{\infty} h_k(f) = B^{-1}f + B^{-1}\sum_{l=2}^{\mathcal{N}}\sum_{k=l}^{\infty}\sum_{j_1+\cdots+j_l=k}\overline{G}_l^{(0)}(h_{j_1},\ldots,h_{j_l})f$$

$$+B^{-1}\sum_{l=2}^{\mathcal{N}}\sum_{k=l}^{\infty}\sum_{j_1+\cdots+j_l=k}[\overline{G}_l^{(0)}(h_{j_1},\ldots,h_{j_l}) - G_l(h_{j_1},\ldots,h_{j_l})]. \tag{43}$$

Double sum $\sum_{l=2}^{\mathcal{N}}\sum_{k=l}^{\infty}$ is transformed as follows

$$\sum_{l=2}^{\mathcal{N}}\sum_{k=l}^{\infty} = \sum_{l=2}^{\mathcal{N}-1}\sum_{k=l}^{\mathcal{N}-1} + \sum_{l=2}^{\mathcal{N}}\sum_{k=\mathcal{N}}^{\infty} = \sum_{k=2}^{\mathcal{N}-1}\sum_{l=2}^{k} + \sum_{k=\mathcal{N}}^{\infty}\sum_{l=2}^{\mathcal{N}} \tag{44a}$$

or as follows

$$\sum_{l=2}^{\mathcal{N}}\sum_{k=l}^{\infty} = \sum_{l=2}^{\mathcal{N}}\sum_{k=l}^{\mathcal{N}} + \sum_{l=2}^{\mathcal{N}}\sum_{k=\mathcal{N}+1}^{\infty} = \sum_{k=2}^{\mathcal{N}}\sum_{l=2}^{k} + \sum_{k=\mathcal{N}+1}^{\infty}\sum_{l=2}^{\mathcal{N}}. \tag{44b}$$

Substituting (44a) and (44b) into (43) we get the relation

$$\sum_{k=1}^{\infty} h_k(f) = B^{-1}f + B^{-1}\sum_{k=3}^{\mathcal{N}}\sum_{l=2}^{k-1}\sum_{j_1+\cdots+j_l=k-1}\overline{G}_l^{(0)}(h_{j_1},\ldots,h_{j_l})f$$

$$+B^{-1}\sum_{k=\mathcal{N}+1}^{\infty}\sum_{l=2}^{\mathcal{N}}\sum_{j_1+\cdots+j_l=k-1}\overline{G}_l^{(0)}(h_{j_1},\ldots,h_{j_l})f$$

$$+B^{-1}\sum_{k=2}^{\mathcal{N}}\sum_{l=2}^{k}\sum_{j_1+\cdots+j_l=k}[\overline{G}_l^{(0)}(h_{j_1},\ldots,h_{j_l}) - G_l(h_{j_1},\ldots,h_{j_l})]$$

$$+B^{-1}\sum_{k=\mathcal{N}+1}^{\infty}\sum_{l=2}^{\mathcal{N}}\sum_{j_1+\cdots+j_l=k}[\overline{G}_l^{(0)}(h_{j_1},\ldots,h_{j_l}) - G_l(h_{j_1},\ldots,h_{j_l})]. \tag{45}$$

Here in the first two sums of the right-hand side we change summation variable k to $k+1$.

In this relation all sums with respect to k contain expressions of order k relative to f. Putting terms of the same order being equal in accordance with the theorem on uniqueness of analytical operators [9] we obtain the next recurrent system for the functions $h_k(f)$

$$h_1(f) = B^{-1}f, \tag{46a}$$

$$h_2(f) = B^{-1}[\overline{G}_2^{(0)}(h_1,h_1) - G_2(h_1,h_1)], \tag{46b}$$

$$h_k(f) = B^{-1}\sum_{l=2}^{k-1}\sum_{j_1+\cdots+j_l=k-1}\overline{G}_l^{(0)}(h_{j_1},\ldots,h_{j_l})f + B^{-1}\sum_{l=2}^{k}\sum_{j_1+\cdots+j_l=k}$$

$$\cdot[\overline{G}_l^{(0)}(h_{j_1},\ldots,h_{j_l}) - G_l(h_{j_1},\ldots,h_{j_l})], \qquad 3 \le k \le \mathcal{N}, \tag{46c}$$

$$h_k(f) = B^{-1}\sum_{l=2}^{\mathcal{N}}\sum_{j_1+\cdots+j_l=k-1}\overline{G}_l^{(0)}(h_{j_1},\ldots,h_{j_l})f + B^{-1}\sum_{l=2}^{\mathcal{N}}\sum_{j_1+\cdots+j_l=k}$$

$$\cdot[\overline{G}_l^{(0)}(h_{j_1},\ldots,h_{j_l}) - G_l(h_{j_1},\ldots,h_{j_l})], \qquad k \ge \mathcal{N}+1. \tag{46d}$$

All terms of series (40) are calculated from this system. So the solution of the equation (15) is founded. It satisfies additional condition (16). Convergence of series (40) with $h_k(f)$ being the solutions of system $(46a)$-$(46d)$ is proved by Cauchy-Goursat method presented in the book [5].

As soon as h_k are expressed in terms of f we can get the canonical distribution (9) in terms of F_s since f and F_s are uniquely connected by relation (11).

5. Calculation procedure for the canonical Gibbs distribution

Since canonical distribution (9) is a ratio of two polynomials with respect to h, we see that D_N is an analytical operator function of h. We have just proved that h is an analytical operator function of f. Therefore D_N is an analytical operator function of f and it can be expanded into an absolutely convergent series relative to f

$$D_N = V^{-N}\Big[1 + \sum_{k=1}^{\infty} \varphi_k(f)\Big], \tag{47}$$

where $\varphi_k(f)$ is a uniform operator of order k transforming function $f(q_1, \dots, q_s)$ to function $\varphi_k(q_1, \dots, q_N; [f])$. Taking into account the definitions of reduced distribution functions (4) and function $f(q_1, \dots, q_s)$ (11) we can get relations for φ_k

$$\frac{1}{V^{N-s}} \int dq_{s+1} \cdots dq_N \varphi_1(q_1, \dots, q_N; [f]) = f(q_1, \dots, q_s), \tag{48}$$

$$\int dq_{s+1} \cdots dq_N \varphi_k(q_1, \dots, q_N; [f]) = 0, \qquad k = 2, 3, \dots. \tag{49}$$

Below we construct a procedure for calculation of functions $\varphi_l(q_1, \dots, q_N; [f])$ in terms of f.

We introduce a nonlinear operator function $\lambda(h)$ by the relation

$$\prod_{1 \le j_1 < \cdots < j_s \le N} [1 + h(q_{j_1}, \dots, q_{j_s})] = 1 + \lambda(h). \tag{50}$$

This operator function is a polynomial of degree $\mathcal{N}$ relative to h. It can be written in the form

$$\lambda(h) = \sum_{k=1}^{\mathcal{N}} \lambda_k(h), \tag{51}$$

where $\lambda_k(h)$ are defined by relations

$$\lambda_k(q_1, \dots, q_N; [h]) = \sum_{1 \le K_1 < \cdots < K_k \le \mathcal{N}} h(X_{K_1}) \cdots h(X_{K_k}). \tag{52}$$

Introduce also multilinear operators

$$\Lambda_k(y_1, \dots, y_k) \stackrel{\text{def}}{=} \sum_{1 \le K_1 < \cdots < K_k \le \mathcal{N}} y_1(X_{K_1}) \cdots y_k(X_{K_k}). \tag{53}$$

It's evident that

$$\lambda_k(h) = \Lambda_k(h, \dots, h). \tag{54}$$

The operators introduced here are connected with the operators $g(h)$, $g_k(h)$, and $G_k(h_1,\ldots,h_k)$ by the relations

$$\frac{1}{V^{N-s}}\int dq_{s+1}\cdots dq_N\lambda(q_1,\ldots,q_N;[h])=g(q_1,\ldots,q_s;[h]), \tag{55}$$

$$\frac{1}{V^{N-s}}\int dq_{s+1}\cdots dq_N\lambda_k(q_1,\ldots,q_N;[h])=g_k(q_1,\ldots,q_s;[h]), \tag{56}$$

$$\frac{1}{V^{N-s}}\int dq_{s+1}\cdots dq_N\Lambda_k(q_1,\ldots,q_N;[h_1,\ldots,h_k])$$
$$=G_k(q_1,\ldots,q_s;[h_1,\ldots,h_k]). \tag{57}$$

In particular for $k=1$

$$\frac{1}{V^{N-s}}\int dq_{s+1}\cdots dq_N\Lambda_1(q_1,\ldots,q_N;[h])$$
$$=G_1(q_1,\ldots,q_s;[h])=g_1(q_1,\ldots,q_s;[h])=(Bh)(q_1,\ldots,q_s). \tag{58}$$

Taking into account the expression (34) for Q_N we can write

$$D_N=V^{-N}\frac{1+\lambda(h)}{1+\overline{g}^{(0)}(h)}. \tag{59}$$

Comparing it with (47) we get the relation

$$\sum_{k=1}^{\infty}\varphi_k(f)=\frac{\lambda(h)-\overline{g}^{(0)}(h)}{1+\overline{g}^{(0)}(h)}, \tag{60}$$

where h is the operator function of f calculated in previous section. Using here the expressions for $\lambda(h)$, $\overline{g}^{(0)}(h)$ and $h(f)$ we can transform the right-hand side of (60) to series with respect to f and thus obtain expressions for $\varphi_k(f)$. But less awkward transformations are obtained if we construct a recurrent system for $\varphi_k(f)$.

Multiplying (60) by $1+\overline{g}^{(0)}(h)$ and using (38) and (54) we obtain

$$\{1+\sum_{k=2}^{\mathcal{N}}\overline{G}_k^{(0)}(h,...,h)\}\sum_{l=1}^{\infty}\varphi_l(f)=\sum_{k=1}^{\mathcal{N}}\Lambda_k(h,...,h)-\sum_{k=2}^{\mathcal{N}}\overline{G}_k^{(0)}(h,...,h). \tag{61}$$

Substitution of the expansion (40) here gives

$$\{1+\sum_{k=2}^{\mathcal{N}}\sum_{j_1=1}^{\infty}\cdots\sum_{j_k=1}^{\infty}\overline{G}_k^{(0)}(h_{j_1},...,h_{j_k})\}\sum_{l=1}^{\infty}\varphi_l(f)$$
$$=\sum_{k=1}^{\mathcal{N}}\sum_{j_1=1}^{\infty}\cdots\sum_{j_k=1}^{\infty}\Lambda_k(h_{j_1},...,h_{j_k})-\sum_{k=2}^{\mathcal{N}}\sum_{j_1=1}^{\infty}\cdots\sum_{j_k=1}^{\infty}\overline{G}_k^{(0)}(h_{j_1},...,h_{j_k}). \tag{62}$$

Further calculation is carried out in the same way as in the previous section. We won't make it and write a recurrent system for $\varphi_k(f)$ straight away

$$\varphi_1(f)=\Lambda_1(h_1), \tag{63a}$$

$$\varphi_2(f)=\Lambda_1(h_2)+\Lambda_2(h_1,h_1)-\overline{G}_2^{(0)}(h_1,h_1), \tag{63b}$$

$$\varphi_k(f)=\Lambda_1(h_k)+\sum_{l=2}^{k}\sum_{j_1+\cdots+j_l=k}\{\Lambda_l(h_{j_1},...,h_{j_l})-\overline{G}_l^{(0)}(h_{j_1},...,h_{j_l})\}$$

$$-\sum_{l=3}^{k}\sum_{j_1+\cdots+j_l=k}\overline{G}_{l-1}^{(0)}(h_{j_1},...,h_{j_{l-1}})\varphi_{j_l}(f), \qquad 3\le k\le\mathcal{N}, \tag{63c}$$

$$\varphi_k(f)=\Lambda_1(h_k)+\sum_{l=2}^{\mathcal{N}}\sum_{j_1+\cdots+j_l=k}\{\Lambda_l(h_{j_1},...,h_{j_l})-\overline{G}_l^{(0)}(h_{j_1},...,h_{j_l})\}$$

$$-\sum_{l=3}^{\mathcal{N}+1}\sum_{j_1+\cdots+j_l=k}\overline{G}_{l-1}^{(0)}(h_{j_1},...,h_{j_{l-1}})\varphi_{j_l}(f), \qquad k\ge\mathcal{N}+1. \tag{63d}$$

In this relations we have to use the expressions for $h_r(f)$ derived from the recurrent system (46a)–(46d).

For example an expression for $\varphi_1(f)$ is

$$\varphi_1(q_1,\dots,q_N;[f])=\sum_{r=1}^{s}(-1)^{s-r}C_{N-r-1}^{s-r}\sum_{1\le j_1<\cdots<j_r\le N}\overline{f}^{(r)}(q_{j_1},\dots,q_{j_r}). \tag{64}$$

It is easy to show that expressions (63a)–(63d) and (64) satisfy conditions (48), (49). For s=2 expression (64) coincides with $\varphi_1(q_1,\dots,q_N;[f])$ derived in the papers [3, 4].

6. Inadequacy of reduced distribution functions of order less then s

Let us test the theorem conditions for reduced l-particle distribution function when $l<s$. Introduce a function $f_l(q_1,\dots,q_l)$ by relation

$$F_l(q_1,\dots,q_l)=\frac{N!}{(N-l)!\,V^l}[1+f_l(q_1,\dots,q_l)]. \tag{65}$$

All constructions and reasonings of sections 2 and 3 remain valid. We obtain the operator equation $\mathcal{F}_l(h,f_l)=0$ and appropriate additional condition. There are proper Banach spaces and bounded operator B_l which is Fréchet derivative of the nonlinear operator $\mathcal{F}_l(h,f_l)$ relative to h. It is easy to show that the operator B_l is resulted by integrating of the operator B with respect to $q_{l+1},\dots,q_s$. Therefore a uniform equation $B_lh=0$ has the form (see derivation of equation (25))

$$\sum_{r=1}^{l}C_{N-l}^{s-r}\sum_{1\le j_1<\cdots<j_r\le l}\overline{h}^{(r)}(q_{j_1},\dots,q_{j_r})=0. \tag{66}$$

From here we see that the operator B_l has a nontrivial space of zeroes. This space consists of all functions $h(q_1,\dots,q_s)\in E_1$ satisfying a condition

$$\int h(q_1,\dots,q_s)dq_{l+1}\cdots dq_s=0 \tag{67}$$

for any fixed l. This means that the operator B_l^{-1} isn't exist as $l<s$ and inverse transformation $\{f_l\to h\}$ isn't exist either. Therefore we can't express the canonical distribution D_N in terms of f_l as $l<s$. As soon as $l=s$ the operator $B_l=B$ and the space of zeroes of operator B_l becomes trivial (see the condition (67)). In this case all conditions of the theorem are valid and we obtain all above results. So the reduced s-particle distribution function plays a specific role for the system with s-body interaction.

F_s is a reduced distribution function of minimal order containing all information about this system.

7. Conclusion

Using the theorem on implicit functions in this article it is shown that a reduced distribution function of order s plays a specific role for a canonical ensemble of N particles with s-body interaction. The canonical Gibbs distribution $D_N(q_1 \ldots, q_N)$ can be expressed uniquely in terms of this function $F_s(q_1 \ldots, q_s)$. From here we easily conclude that there is a one-to-one correspondence between these two functions. This means that the reduced distribution function F_s contains information about system under consideration as much as the whole canonical distribution D_N. Reduced distribution functions of all orders can be expressed in terms of this single function F_s.

All reduced distribution functions of order l less then s don't satisfy the theorem conditions. So it is impossible to express the canonical distribution in terms of these functions of order $l < s$. To all appearance they contain not all information about the system under consideration.

Considered theorem provides sufficient conditions for existence and uniqueness of inverse transformation $\{f \to h\}$. Results obtained here are valid in some neighbourhood of $h^{(0)} = 0$, $f^{(0)} = 0$. The question about size of this neighbourhood demands special investigation.

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